Crossover temperature of Bose-Einstein condensation in an atomic Fermi gas

G.M. Falco[1] and H.T.C. Stoof[1]

[1] *Institute for Theoretical Physics, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands*

We show that in an atomic Fermi gas near a Feshbach resonance the crossover between a Bose-Einstein condensate of diatomic molecules and a Bose-Einstein condensate of Cooper pairs occurs at positive detuning, i.e., when the molecular energy level lies in the two-atom continuum. We determine the crossover temperature as a function of the applied magnetic field and find excellent agreement with the experiment of Regal *et al.* [Phys. Rev. Lett. **92**, 040403 (2004)] that has recently observed this crossover temperature.

Introduction. — An atomic Fermi gas near a Feshbach resonance is a fundamentally new superfluid system. The reason is that near a Feshbach resonance the gas does not only consist of atoms but also of diatomic molecules. Moreover, the energy difference between the molecular level and the threshold of the two-atom continuum, known as the detuning δ, can be experimentally tuned by means of a magnetic field [1, 2]. In combination with the fact that for fermionic atoms these molecules are very long lived [3, 4, 5, 6], such a gas thus offers the exciting opportunity to study in detail the crossover between the Bose-Einstein condensation (BEC) of diatomic molecules and the Bose-Einstein condensation of atomic Cooper pairs, i.e., the Bardeen-Cooper-Schrieffer (BCS) transition [7, 8, 9, 10]. Indeed, a Bose-Einstein condensate of molecules has recently been observed [11, 12, 13]. More recently, a claim for Bose-Einstein condensation of atomic Cooper pairs was made [14]. We will show, however, that the date reported in Ref. [14] can be understood in terms of a Bose-Einstein condensation of molecules.

At zero temperature the physics of the BEC-BCS crossover occurring near a Feshbach resonance can be understood as follows. The superfluid phase of the gas is always associated with a Bose-Einstein condensate of pairs of atoms, but the wave function of the pairs is given by

$$\sqrt{Z(\delta)}\chi_{\rm m}(\mathbf{x},\mathbf{x}')|{\rm closed}\rangle + \sqrt{1-Z(\delta)}\chi_{\rm aa}(\mathbf{x},\mathbf{x}';\delta)|{\rm open}\rangle \ .$$

At large negative detuning the energy of the molecule lies far below the threshold of the two-atom continuum and we have $Z(\delta) \simeq 1$. In that case we are dealing with a Bose-Einstein condensate of diatomic molecules and the spatial part of the pair wave function is equal to the (bare) molecular wave function $\chi_{\rm m}(\mathbf{x},\mathbf{x}')$. The spin part of the pair wave function is then equal to $|{\rm closed}\rangle$, i.e., the spin state of the closed channel of the relevant Feshbach problem [15]. At large positive detuning the molecular energy level lies far above the threshold of the two-atom continuum and can be (adiabatically) eliminated. We then have that $Z(\delta) \simeq 0$ and the spatial part of the pair wave function equals the usual BCS wave function for atomic Cooper pairs $\chi_{\rm aa}(\mathbf{x},\mathbf{x}';\delta)$. This Cooper-pair wave function depends on the detuning, because the effective attraction between the atoms depends on the detuning. The spin state of the Cooper pairs is, however, always equal to the spin state of the open channel of the Feshbach problem, denoted here by $|{\rm open}\rangle$.

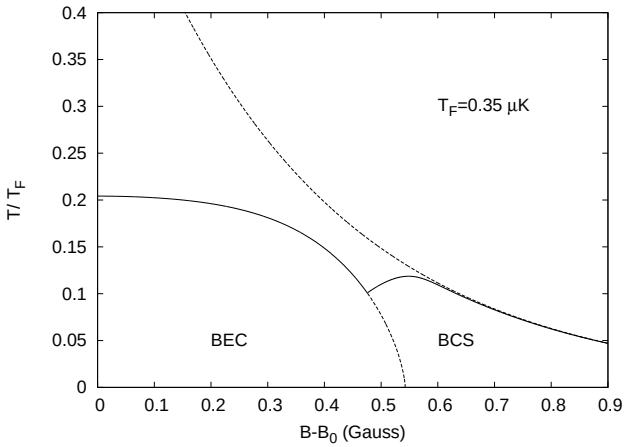

FIG. 1: Phase diagram of atomic ^{40}K as a function of magnetic field and temperature for a Fermi temperature of the gas of $T_{\rm F} = 0.35$ μK. The solid line gives the critical temperature for either a Bose-Einstein condensation of molecules or a Bose-Einstein condensation of atomic Cooper pairs. The critical temperature for the latter is calculated by simultaneously solving the BCS gap equation and the equation of state of an ideal mixture of atoms and molecules. In this equation of state, we use the energy of the molecules given by Eq. (4) below. For comparison, the upper dashed curve is the analytical BCS result $T/T_F = (8e^{\gamma-2}/\pi)e^{-\pi/2k_{\rm F}|a|}$, where $\gamma \simeq 0.5772$ is Euler's constant [7, 18]. The lower dashed line is the crossover between the two Bose-Einstein condensed phases, which is the main topic of this Letter.

With this physical picture in mind, the point where the crossover takes place is thus determined by the detuning at which the amplitude $Z(\delta)$ relatively abruptly crosses over from one to zero. Based on two-body physics [15] we would expect the crossover to occur exactly on resonance, i.e., at zero detuning. It is the main purpose of this Letter, however, to point out that many-body physics changes this result and shifts the crossover point to positive detuning. Quantitatively, the crossover oc-

curs, for an incoherent mixture of two hyperfine states with equal density $n/2$, at the detuning where the molecular energy level becomes equal to twice the Fermi energy $\epsilon_{\rm F} = \hbar^2(3\pi^2 n)^{2/3}/2m$. Using the theory presented below we can also accurately determine the crossover point at nonzero temperatures. The resulting (mean-field) phase diagram for atomic ^{40}K under the conditions of the experiment of Regal *et al.* is shown in Fig. 1 and summarizes the main conclusion of our work.

Note that in the usual BEC-BCS crossover problem, studied in condensed-matter physics in the context of the high-temperature superconductors, $Z(\delta)$ is always identically zero and the crossover is associated with a qualitatively different behavior of the Cooper-pair wave function $\chi_{\rm aa}(\mathbf{x}, \mathbf{x}'; \delta)$ [16, 17, 18]. This emphasizes the fundamentally new nature of the superfluid state in an atomic Fermi gas near a Feshbach resonance, which actually shows a macroscopic coherence between atoms and molecules.

Poor man's approach. — Before discussing the theory that incorporates the resonant interactions between atoms, we first consider the case of an ideal mixture of molecules and atoms to establish the physical picture of the crossover most clearly. At positive detuning a stable molecular state does not exist, because the molecule can energetically decay into two free atoms. In previous work [15, 19], however, we have shown that in first instance it is reasonably accurate to neglect the finite lifetime of the molecule. Close to the Feshbach resonance, the interaction with the atomic continuum shifts the molecular energy level downward from the detuning δ to $\epsilon_{\rm m} \simeq \hbar^2/ma^2$. Here $a(B) = a_{\rm bg}[1-\Delta B/(B-B_0)]$ is the full atomic s-wave scattering length of the Feshbach resonance, which is experimentally characterized by its location at magnetic field B_0, its magnetic field width ΔB, and the background scattering length $a_{\rm bg}$.

If the molecules are Bose-Einstein condensed, the chemical potential of the atoms is equal to $\epsilon_{\rm m}/2 \simeq \hbar^2/2ma^2$. If we take the atoms to be noninteracting, we can thus at zero temperature immediately determine the density of atoms in the Fermi sea below the chemical potential. Subtracting this result from the total density n, and dividing by two, we find that at zero temperature the density of molecules in the Bose-Einstein condensate is equal to

$$n_{\rm mc} \simeq \frac{n}{2}\left[1 - \frac{1}{(k_{\rm F}|a|)^3}\right] , \qquad (1)$$

where $k_{\rm F} = (3\pi^2 n)^{1/3}$ is the Fermi momentum of the gas. Note that this estimate is only valid for positive detuning, where $a < 0$. So at resonance the density of condensed molecules is just n/2, i.e., half the total density of atoms in the gas. Moreover, the density of condensed molecules vanishes at $k_F|a| = 1$. Physically, this situation occurs when the energy level of the molecule is exactly equal to twice the Fermi energy of the gas. This result is sensible, since if the energy level of the molecule is higher, there will be no molecules at zero temperature. The whole gas then consists of atoms. In the experiment of Regal *et al.*, this condition gives a magnetic field of 0.5 Gauss above the resonance, in excellent agreement with the data shown in their Fig. 2.

To find the same criterion at nonzero temperatures is also possible. We know that for temperatures below the Fermi temperature the density of fermionic atoms is hardly influenced by temperature. Not too close to resonance the molecular condensate density is just depleted by thermal fluctuations, i.e., a thermal cloud of molecules forms with increasing temperature. Calculating the critical temperature for a density of ideal Bose molecules given by Eq. (1) gives us the result

$$\frac{T}{T_{\rm F}} \simeq 2\pi \left\{ \frac{1}{6\pi^2\zeta(3/2)}\left[1 - \frac{1}{(k_{\rm F}|a|)^3}\right]\right\}^{2/3} , \qquad (2)$$

with $T_{\rm F} = \epsilon_{\rm F}/k_{\rm B}$ the Fermi temperature and $\zeta(3/2) \simeq 2.612$. This result can be directly compared with the data of Regal *et al.* presented in the x-y plane of their Fig. 4. In view of the simplicity of the approach, the agreement is remarkable.

Molecular Bose-Einstein condensate. — To properly incorporate the resonant interactions between the atoms, a more involved treatment of the gas is necessary. Introducing creation and annihilation operators for the molecules and atoms, the grand-canonical hamiltonian of the gas becomes [20]

$$\begin{aligned} H = &\int dx \psi_{\rm m}^\dagger(x)\left[-\frac{\hbar^2\nabla^2}{4m} + \epsilon_{\rm m} - 2\mu\right]\psi_{\rm m}(x) \\ &+ \sum_{\sigma=\uparrow,\downarrow}\int dx \psi_\sigma^\dagger(x)\left[-\frac{\hbar^2\nabla^2}{2m} - \mu\right]\psi_\sigma(x) \\ &+ \int dx g\left[\psi_{\rm m}^\dagger(x)\psi_\uparrow(x)\psi_\downarrow(x) + \psi_\downarrow^\dagger(x)\psi_\uparrow^\dagger(x)\psi_{\rm m}(x)\right] , \end{aligned} \qquad (3)$$

where the two hyperfine state of the atoms are denoted by $|\uparrow\rangle$ and $|\downarrow\rangle$, the atom-molecule coupling constant $g = \hbar\sqrt{4\pi a_{\rm bg}\Delta B \Delta\mu_{\rm mag}/m}$, and the magnetic moment difference $\Delta\mu_{\rm mag}$ between the hyperfine states $|{\rm open}\rangle \equiv (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ and $|{\rm closed}\rangle$ gives the detuning $\delta = \Delta\mu_{\rm mag}(B - B_0)$ [21]. Finally, the molecular energy is approximated by the energy where the molecular density of states has a maximum. To find this maximum we use that in the two-body T-matrix approximation the frequency-dependent self-energy of the molecules is $-i\eta\sqrt{\hbar\omega}$ [15, 20]. In general, this gives

$$\epsilon_{\rm m} = \frac{1}{3}\left(\delta - \frac{\eta^2}{2} + \sqrt{\frac{\eta^4}{4} - \eta^2\delta + 4\delta^2}\right) , \qquad (4)$$

where $\eta^2 = g^4m^3/16\pi^2\hbar^6$ is the energy scale associated with the width of the Feshbach resonance. This energy scale is in fact of fundamental importance, because it

shows that at zero temperature the thermodynamic properties of a resonant atomic Fermi are not solely determined by the Fermi energy. This is particularly true for the experiment of Regal *et al.*, for which $\eta^2 \gg \epsilon_{\rm F}$, since for the Feshbach resonance of interest $\eta^2 \simeq 7.7$ mK. Close to resonance, where $\delta \ll \eta^2$, the molecular energy reduces to δ^2/η^2, which can be shown to be equivalent to $\hbar^2/ma^2$ as expected. Note that the omission of the background scattering length in the hamiltonian is justified because the region of interest takes place relatively close to resonance.

To find the crossover temperature for positive detuning, we consider the gas to have a Bose-Einstein condensate of molecules, and perform a quadratic expansion of the hamiltonian around the nonzero expectation value $\langle\psi_{\rm m}(\mathbf{x})\rangle \equiv \sqrt{n_{\rm mc}}$. This leads to the ideal gas expression for the molecular density

$$n_{\rm m} = n_{\rm mc} + \frac{1}{V}\sum_{\mathbf{k}} \frac{1}{e^{\epsilon_{\mathbf{k}}/2k_{\rm B}T} - 1} \ , \qquad (5)$$

where V is the volume of the gas and $\epsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m$. However, for atoms with momentum $\mathbf{k}$, the resulting hamiltonian leads to a fluctuation matrix

$$\begin{bmatrix} \epsilon_{\mathbf{k}} - \epsilon_{\rm m}/2 & g\sqrt{n_{\rm mc}} \\ g\sqrt{n_{\rm mc}} & -(\epsilon_{\mathbf{k}} - \epsilon_{\rm m}/2) \end{bmatrix} \ ,$$

which can easily be diagonalized by means of a Bogoliubov transformation. Performing the calculation, we ultimately find for the total atomic density

$$n_{\rm a} = \frac{2}{V}\sum_{\mathbf{k}} \left(\frac{\epsilon_{\mathbf{k}} - \epsilon_{\rm m}/2}{\hbar\omega_{\mathbf{k}}} \frac{1}{e^{\hbar\omega_{\mathbf{k}}/k_{\rm B}T} + 1} + \frac{\hbar\omega_{\mathbf{k}} - \epsilon_{\mathbf{k}} + \epsilon_{\rm m}/2}{2\hbar\omega_{\mathbf{k}}} \right) , \qquad (6)$$

where the dispersion for the atoms obeys $\hbar\omega_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \epsilon_{\rm m}/2)^2 + g^2 n_{\rm mc}}$.

For fixed positive detuning and temperature, the equation for the total atomic density $n = 2n_{\rm m} + n_{\rm a}$ determines the molecular condensate $n_{\rm mc}$. The result of these calculations for the experiment of Regal *et al.* is shown in Fig. 2. This figure can be directly compared with the data in their Fig. 4. Again the agreement is remarkable. Having said that, it is important to realize that the experiment is performed in an optical trap, whereas we have considered the homogeneous situation. Generalizing our poor man's approach to the trapped situation shows, however, that this does not affect the position of the crossover line, because in that case the homogeneous criterion is satisfied in the center of the trap. The inhomogeneous analysis can be carried out in the local-density (or Thomas-Fermi) approximation, but this is beyond the scope of the present paper and is left for future work. Such an analysis is certainly needed to obtain a full quantitative agreement between theory and experiment.

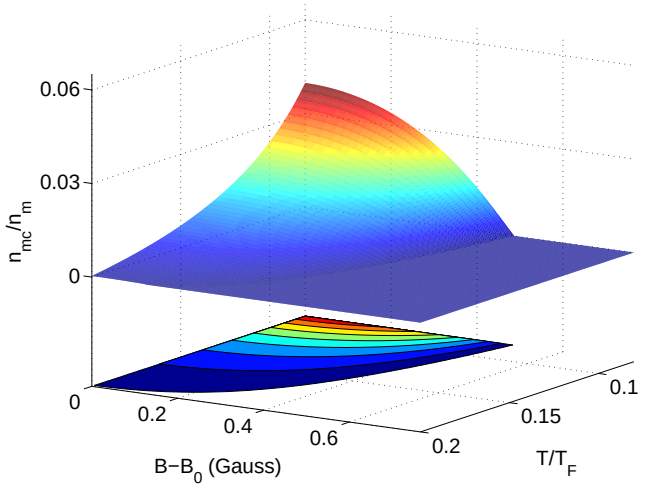

FIG. 2: Molecular condensate fraction $n_{\rm mc}/n_{\rm m}$ in an atomic ^{40}K gas as a function of magnetic field and temperature for a Fermi temperature of the gas of $T_{\rm F} = 0.35\mu$K. This figure should be compared with Fig. 4 of Ref. [14].

The most important approximation that we have made in our calculation of the crossover temperature is to neglect the finite lifetime of the molecules. Including this finite lifetime is not an easy task, because a consistent approach requires that the self-energy of the molecules is calculated at least in the many-body T-matrix approximation, just as we have done in our recent work on the observation of molecular Kondo resonances in an atomic Fermi gas near a Feshbach resonance [20]. The physical reason for this complication is that the decay of the molecules can be Pauli blocked by the presence of the atomic Fermi sea. It is this Pauli blocking that is ultimately responsible for the molecular Kondo resonances and it will, therefore, also play an important role in a quantitative analysis of the molecular lifetime effects. Qualitatively, we expect that a broadening of the molecular energy level will not have a substantial effect on the location of the crossover line. It will, however, lead to an increase of the molecular condensate fraction, because of the presence of molecular states with energies below $\epsilon_{\rm m}$. We believe that these lifetime effects may also have a bearing on the considerable narrowing of the molecular thermal cloud that was also observed by Regal *et al.* [14]. Work in this direction is presently being completed and will be reported elsewhere.

We thank Randy Hulet for numerous stimulating discussions that have lead us to the above. This work is supported by the Stichting voor Fundamenteel Onderzoek der Materie (FOM) and the Nederlandse Organisatie voor Wetenschaplijk Onderzoek (NWO).

[1] W. C. Stwalley, Phys. Rev. Lett. **37**, 1628 (1976).

[2] E. Tiesinga, B. J. Verhaar, and H. T. C. Stoof, Phys. Rev. A **47**, 4114 (1993).

[3] D. S. Petrov, Phys. Rev. A **67**, 010703 (2003).

[4] K. E. Strecker, G. B. Partridge, and R. G. Hulet, Phys. Rev. Lett. **91**, 080406 (2003).

[5] J. Cubizolles, T. Bourdel, S. J. J. M. F. Kokkelmans, G. V. Shlyapnikov, and C. Salomon, Phys. Rev. Lett. **91**, 240401 (2003).

[6] S. Jochim, M. Bartenstein, A. Altmeyer, G. Hendl, C. Chin, J. H. Denschlag, and R. Grimm, Phys. Rev. Lett. **91**, 240402 (2003).

[7] H. T. C. Stoof, M. Houbiers, C. A. Sackett, and R. G. Hulet, Phys. Rev. Lett. **76**, 10 (1996).

[8] E. Timmermans, K. Furuya, P. W. Milonni, and A. K. Kerman, Phys. Lett. A **285**, 228 (2001).

[9] Y. Ohashi and A. Griffin, Phys. Rev. Lett. **89**, 130402 (2002); Phys. Rev. A **67**, 033603 (2003); Phys. Rev. A **67**, 063612 (2003).

[10] J. N. Milstein, S. J. J. M. F. Kokkelmans and M. J. Holland, Phys. Rev. A **66**, 043604 (2002).

[11] S. Jochim, M. Bartenstein, A. Altmeyer, G. Hendl, S. Riedl, C. Chin, J. H. Denschlag, and R. Grimm, Science **302**, 2101 (2003).

[12] M. Greiner, C. A. Regal, and D. S. Jin, Nature **426**, 537 (2003).

[13] M. W. Zwierlein, C. A. Stan, C. H. Schunck, S. M. F. Raupach, S. Gupta, Z. Hadzibabic, W. Ketterle, Phys. Rev. Lett. **91**, 250401 (2003).

[14] C. A. Regal, M. Greiner, and D. S. Jin, Phys. Rev. Lett. **92**, 040403 (2004).

[15] For a recent review see R. A. Duine and H. T. C. Stoof (cond-mat/0312254).

[16] A. J. Leggett, J. Phys. C. (Paris) **41**, 7 (1980).

[17] P. Nozières and S. Schmitt-Rink, J. Low Temp. Phys. 59, 195 (1985).

[18] C. A. R. Sáde Melo, M. Randeria, and J. R. Engelbrecht, Phys. Rev. Lett. 71, 3202 (1993).

[19] R. A. Duine and H. T. C. Stoof, J. Opt. B: Quantum Semiclass. Opt. **5**, S212 (2003).

[20] G. M. Falco, R. A. Duine, and H. T. C. Stoof, Phys. Rev. Lett. **92** (2004) (cond-mat/0304489).

[21] Since the label σ of the hyperfine states $|\sigma\rangle$ does not correspond to the electron spin of the atom, the open channel of a Feshbach resonance is actually never a singlet, but usually contains mostly a triplet component. As a result we almost always have that $\Delta\mu_{\rm mag} \simeq 2\mu_{\rm B}$, with $\mu_{\rm B}$ the Bohr magneton.